Felix Plasser

List of Publications by Year in Descending Order

100 papers	5,467 citations	34 h-index	73 g-index
124 ext. papers	6,635 ext. citations	5.7 avg, IF	6.37 L-index

#	Paper	IF	Citations
100	Sterically demanding macrocyclic Eu(iii) complexes for selective recognition of phosphate and real-time monitoring of enzymatically generated adenosine monophosphate.. *Chemical Science*, **2022**, 13, 3386-3394	9.4	0
99	The role of excited-state character, structural relaxation, and symmetry breaking in enabling delayed fluorescence activity in push-pull chromophores. *Physical Chemistry Chemical Physics*, **2021**, 23, 26135-26150	3.6	2
98	Identifying the Trade-off between Intramolecular Singlet Fission Requirements in Donor–Acceptor Copolymers. *Chemistry of Materials*, **2021**, 33, 2567-2575	9.6	5
97	Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies. *Journal of Physical Chemistry Letters*, **2021**, 12, 2712-2720	6.4	13
96	Mechanistic insight into the fluorescence activity of forensic fingerprinting reagents. *Journal of Chemical Physics*, **2021**, 154, 124313	3.9	1
95	Excited-state dynamics of [Mn(im)(CO)(phen)]: PhotoCORM, catalyst, luminescent probe?. *Journal of Chemical Physics*, **2021**, 154, 154102	3.9	2
94	Exploitation of Baird Aromaticity and Clar's Rule for Tuning the Triplet Energies of Polycyclic Aromatic Hydrocarbons. *Chemistry*, **2021**, 3, 532-549	2.1	6
93	Visualisation of Chemical Shielding Tensors (VIST) to Elucidate Aromaticity and Antiaromaticity. *European Journal of Organic Chemistry*, **2021**, 2021, 2529-2539	3.2	7
92	Pushing the Limits of the Donor-Acceptor Copolymer Strategy for Intramolecular Singlet Fission. *Journal of Physical Chemistry Letters*, **2021**, 12, 7270-7277	6.4	3
91	Oxygen harvesting from carbon dioxide: simultaneous epoxidation and CO formation. *Chemical Science*, **2021**, 12, 13373-13378	9.4	0
90	Excited-state symmetry breaking in 9,10-dicyanoanthracene-based quadrupolar molecules: the effect of donor-acceptor branch length. *Physical Chemistry Chemical Physics*, **2021**, 23, 15150-15158	3.6	4
89	Highly sensitive 26Al measurements by Ion-Laser-InterAction Mass Spectrometry. *International Journal of Mass Spectrometry*, **2021**, 465, 116576	1.9	4
88	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
87	Surface Hopping Dynamics on Vibronic Coupling Models. *Accounts of Chemical Research*, **2021**, 54, 3760-3771	17.1	8
86	Functional group introduction and aromatic unit variation in a set of π-conjugated macrocycles: revealing the central role of local and global aromaticity. *Organic Chemistry Frontiers*, **2021**, 8, 4730-4745	5.2	4
85	Direct, Mediated, and Delayed Intramolecular Singlet Fission Mechanism in Donor-Acceptor Copolymers. *Journal of Physical Chemistry Letters*, **2020**, 11, 9788-9794	6.4	7
84	Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. *Chemical Science*, **2020**, 11, 7685-7693	9.4	6

83	Multi-Tier Electronic Structure Analysis of Sita's Mo and W Complexes Capable of Thermal or Photochemical N2 Splitting. *European Journal of Inorganic Chemistry*, **2020**, 2020, 1506-1518	2.3	6
82	Solution processed CZTS solar cells using amine–thiol systems: understanding the dissolution process and device fabrication. *Journal of Materials Chemistry C*, **2020**, 8, 10309-10318	7.1	2
81	Toward an understanding of electronic excitation energies beyond the molecular orbital picture. *Physical Chemistry Chemical Physics*, **2020**, 22, 6058-6080	3.6	37
80	TheoDORE: A toolbox for a detailed and automated analysis of electronic excited state computations. *Journal of Chemical Physics*, **2020**, 152, 084108	3.9	95
79	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110	3.9	22
78	A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. *Journal of Materials Chemistry C*, **2020**, 8, 7793-7804	7.1	12
77	Multi-Reference Configuration Interaction **2020**, 277-297		1
76	Designing Singlet Fission Candidates from Donor–Acceptor Copolymers. *Chemistry of Materials*, **2020**, 32, 6515-6524	9.6	16
75	A complementary approach to conjugated -acyliminium formation through photoredox-catalyzed intermolecular radical addition to allenamides and allencarbamates. *Beilstein Journal of Organic Chemistry*, **2020**, 16, 1983-1990	2.5	3
74	Annihilation Dynamics of Molecular Excitons Measured at a Single Perturbative Excitation Energy. *Journal of Physical Chemistry Letters*, **2020**, 11, 7776-7781	6.4	6
73	Optical absorption properties of metal-organic frameworks: solid state molecular perspective. *Physical Chemistry Chemical Physics*, **2020**, 22, 19512-19521	3.6	8
72	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
71	Dynamics of benzene excimer formation from the parallel-displaced dimer. *Physical Chemistry Chemical Physics*, **2019**, 21, 13916-13924	3.6	16
70	Effect of symmetric and asymmetric substitution on the optoelectronic properties of 9,10-dicyanoanthracene. *Molecular Systems Design and Engineering*, **2019**, 4, 951-961	4.6	10
69	Red-shifted delayed fluorescence at the expense of photoluminescence quantum efficiency - an intramolecular charge-transfer molecule based on a benzodithiophene-4,8-dione acceptor. *Physical Chemistry Chemical Physics*, **2019**, 21, 10580-10586	3.6	10
68	The Influence of the Electronic Structure Method on Intersystem Crossing Dynamics. The Case of Thioformaldehyde. *Journal of Chemical Theory and Computation*, **2019**, 15, 3470-3480	6.4	19
67	Strong Influence of Decoherence Corrections and Momentum Rescaling in Surface Hopping Dynamics of Transition Metal Complexes. *Journal of Chemical Theory and Computation*, **2019**, 15, 5031-5045	6.4	34
66	Computational Assessment of MLCT versus MC Stabilities in First-to-Third-Row d Pseudo-Octahedral Transition Metal Complexes. *Journal of Computational Chemistry*, **2019**, 40, 2377-2390	3.5	4

65	Visualisation of Electronic Excited-State Correlation in Real Space. *ChemPhotoChem*, **2019**, 3, 702-706	3.3	11
64	Excited-State Reactivity of [Mn(im)(CO) (phen)] : A Structural Exploration. *Journal of Computational Chemistry*, **2019**, 40, 72-81	3.5	5
63	Highly efficient surface hopping dynamics using a linear vibronic coupling model. *Physical Chemistry Chemical Physics*, **2018**, 21, 57-69	3.6	55
62	Quantitative wave function analysis for excited states of transition metal complexes. *Coordination Chemistry Reviews*, **2018**, 361, 74-97	23.2	81
61	Benchmarking Excited-State Calculations Using Exciton Properties. *Journal of Chemical Theory and Computation*, **2018**, 14, 710-725	6.4	97
60	Interstate vibronic coupling constants between electronic excited states for complex molecules. *Journal of Chemical Physics*, **2018**, 148, 124119	3.9	21
59	Multireference Approaches for Excited States of Molecules. *Chemical Reviews*, **2018**, 118, 7293-7361	68.1	181
58	Ultrafast Intersystem Crossing vs Internal Conversion in Diimine Transition Metal Complexes: Quantum Evidence. *Journal of Physical Chemistry Letters*, **2018**, 9, 5189-5195	6.4	24
57	Wavelength-optimized Two-Photon Polymerization Using Initiators Based on Multipolar Aminostyryl-1,3,5-triazines. *Scientific Reports*, **2018**, 8, 17273	4.9	23
56	Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. *Journal of Chemical Theory and Computation*, **2018**, 14, 6139-6148	6.4	22
55	Ultrafast Electronic Energy Transfer in an Orthogonal Molecular Dyad. *Journal of Physical Chemistry Letters*, **2017**, 8, 1086-1092	6.4	23
54	Universal Exciton Size in Organic Polymers is Determined by Nonlocal Orbital Exchange in Time-Dependent Density Functional Theory. *Journal of Physical Chemistry Letters*, **2017**, 8, 1205-1210	6.4	34
53	Ultrafast Excited-State Decays in [Re(CO)(N,N)(L)]: Nonadiabatic Quantum Dynamics. *Journal of Chemical Theory and Computation*, **2017**, 13, 1293-1306	6.4	42
52	UV absorption in metal decorated boron nitride flakes: a theoretical analysis of excited states. *Molecular Physics*, **2017**, 115, 2469-2477	1.7	4
51	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptor-Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. *Journal of Chemical Theory and Computation*, **2017**, 13, 2612-2622	6.4	10
50	Electronic delocalization, charge transfer and hypochromism in the UV absorption spectrum of polyadenine unravelled by multiscale computations and quantitative wavefunction analysis. *Chemical Science*, **2017**, 8, 5682-5691	9.4	61
49	Evaluation of the quasi correlated tight-binding (QCTB) model for describing polyradical character in polycyclic hydrocarbons. *Journal of Chemical Physics*, **2017**, 146, 064106	3.9	15
48	Color Fine-Tuning of Optical Materials Through Rational Design. *ChemPhysChem*, **2017**, 18, 549-563	3.2	11

47	Excited-states of a rhenium carbonyl diimine complex: solvation models, spin-orbit coupling, and vibrational sampling effects. *Physical Chemistry Chemical Physics*, **2017**, 19, 27240-27250	3.6	36
46	Detailed Wave Function Analysis for Multireference Methods: Implementation in the Molcas Program Package and Applications to Tetracene. *Journal of Chemical Theory and Computation*, **2017**, 13, 5343-5353	6.4	32
45	Chromophores from hexeneuronic acids: identification of HexA-derived chromophores. *Cellulose*, **2017**, 24, 3671-3687	5.5	18
44	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. *Journal of Chemical Physics*, **2017**, 147, 184109	3.9	23
43	Nonadiabatic Dynamics of Cycloparaphenylenes with TD-DFTB Surface Hopping. *Journal of Chemical Theory and Computation*, **2017**, 13, 5846-5860	6.4	33
42	Charge-transfer states in triazole linked donor-acceptor materials: strong effects of chemical modification and solvation. *Physical Chemistry Chemical Physics*, **2017**, 19, 18055-18067	3.6	14
41	Challenges in Simulating Light-Induced Processes in DNA. *Molecules*, **2017**, 22, 49	4.8	13
40	Description of excited states in [Re(Imidazole)(CO)3 (Phen)](+) including solvent and spin-orbit coupling effects: Density functional theory versus multiconfigurational wavefunction approach. *Journal of Computational Chemistry*, **2016**, 37, 2454-66	3.5	27
39	Excitons in poly(para phenylene vinylene): a quantum-chemical perspective based on high-level ab initio calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 2548-63	3.6	47
38	Polyradical Character of Triangular Non-Kekulé Structures, Zethrenes, p-Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. *Journal of Physical Chemistry A*, **2016**, 120, 1625-36	2.8	70
37	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. *Journal of Chemical Theory and Computation*, **2016**, 12, 1207-19	6.4	100
36	Entanglement entropy of electronic excitations. *Journal of Chemical Physics*, **2016**, 144, 194107	3.9	33
35	Communication: Unambiguous comparison of many-electron wavefunctions through their overlaps. *Journal of Chemical Physics*, **2016**, 145, 021103	3.9	17
34	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
33	Electronic and Photophysical Properties of [Re (L)(CO)3(phen)](+) and [Ru(L)2(bpy)2](2+) (L = imidazole), Building Units for Long-Range Electron Transfer in Modified Blue Copper Proteins. *Journal of Physical Chemistry A*, **2016**, 120, 6934-43	2.8	16
32	High-level ab initio computations of the absorption spectra of organic iridium complexes. *Journal of Physical Chemistry A*, **2015**, 119, 1023-36	2.8	29
31	Electronic excitation processes in single-strand and double-strand DNA: a computational approach. *Topics in Current Chemistry*, **2015**, 356, 1-37		17
30	Exciton size and binding energy limitations in one-dimensional organic materials. *Journal of Chemical Physics*, **2015**, 143, 244905	3.9	31

29	Communication: Exciton analysis in time-dependent density functional theory: How functionals shape excited-state characters. *Journal of Chemical Physics*, **2015**, 143, 171101	3.9	68
28	Statistical analysis of electronic excitation processes: Spatial location, compactness, charge transfer, and electron-hole correlation. *Journal of Computational Chemistry*, **2015**, 36, 1609-20	3.5	78
27	Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the State. *Journal of Physical Chemistry A*, **2015**, 119, 6232-43	2.8	46
26	New tools for the systematic analysis and visualization of electronic excitations. I. Formalism. *Journal of Chemical Physics*, **2014**, 141, 024106	3.9	290
25	New tools for the systematic analysis and visualization of electronic excitations. II. Applications. *Journal of Chemical Physics*, **2014**, 141, 024107	3.9	172
24	Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 1395-405	6.4	139
23	A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	51
22	Newton-X: a surface-hopping program for nonadiabatic molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 26-33	7.9	280
21	Exciton analysis of many-body wave functions: Bridging the gap between the quasiparticle and molecular orbital pictures. *Physical Review A*, **2014**, 90,	2.6	105
20	Study of the diradicaloid character in a prototypical pancake-bonded dimer: the stacked tetracyanoethylene (TCNE) anion dimer and the neutral K(2)TCNE(2) complex. *ChemPhysChem*, **2014**, 15, 165-76	3.2	39
19	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. *Journal of Chemical Physics*, **2014**, 141, 074105	3.9	24
18	Electronic excitation and structural relaxation of the adenine dinucleotide in gas phase and solution. *Photochemical and Photobiological Sciences*, **2013**, 12, 1440-52	4.2	43
17	The multiradical character of one- and two-dimensional graphene nanoribbons. *Angewandte Chemie - International Edition*, **2013**, 52, 2581-4	16.4	168
16	Synthesis, spectroscopy, and computational analysis of photoluminescent bis(aminophenyl)-substituted thiophene derivatives. *ChemPhysChem*, **2013**, 14, 1016-24	3.2	15
15	Electronically excited states in poly(p-phenylenevinylene): vertical excitations and torsional potentials from high-level ab initio calculations. *Journal of Physical Chemistry A*, **2013**, 117, 2181-9	2.8	59
14	Der Multiradikalcharakter ein- und zweidimensionaler Graphen-Nanob□der. *Angewandte Chemie*, **2013**, 125, 2641-2644	3.6	21
13	Electronically excited states and photodynamics: a continuing challenge. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	69
12	Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 2777-89	6.4	284

11	UV absorption spectrum of alternating DNA duplexes. Analysis of excitonic and charge transfer interactions. *Journal of Physical Chemistry A*, **2012**, 116, 11151-60	2.8	61
10	The effect of hydrogen bonding on the excited-state proton transfer in 2-(2'-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. *Physical Chemistry Chemical Physics*, **2012**, 14, 9016-25	3.6	60
9	Surface hopping dynamics using a locally diabatic formalism: charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. *Journal of Chemical Physics*, **2012**, 137, 22A514	3.9	139
8	Electronically excited states and photodynamics: a continuing challenge **2012**, 147-160		1
7	Semiclassical dynamics simulations of charge transport in stacked □ systems. *Journal of Chemical Physics*, **2011**, 134, 034309	3.9	27
6	Excited-state diproton transfer in [2,2'-bipyridyl]-3,3'-diol: the mechanism is sequential, not concerted. *Journal of Physical Chemistry A*, **2009**, 113, 8490-9	2.8	96
5	OpenMolcas: From Source Code to Insight		4
4	[2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(p-phenylene vinylene)s (PPVs). *Open Research Europe*,1, 111		1
3	[2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(p-phenylene vinylene)s (PPVs). *Open Research Europe*,1, 111		0
2	Donor□Acceptor□Donor □Hot Exciton□Triads for High Reverse Intersystem Crossing in OLEDs. *Advanced Optical Materials*,2200509	8.1	0
1	Spin-density calculation via the graphical unitary group approach. *Molecular Physics*,	1.7	1